

Marius STAN, Ph.D.

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PROFESSIONAL SKILLS

MODELS AND SIMULATIONS: Atomistic and continuum thermodynamics, phase stability and phase transformations, phase diagram calculations (CALPHAD), heat and mass transfer simulations (Telluride), kinetics of chemical reactions, and computer optimization of technological flows.

EXPERIMENTAL: X-ray diffraction (XRD), Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), Scanning and Transmission Electronic Microscopy (SEM, TEM).

STUDIED SYSTEMS: U-Pu(Ce)-Ga(Al, Cr, Fe)-O, U-Pu-N, Pu-(Ga, Al, Fe), U-Nb, Pd-H, Sb-Sn-O, Bi-Sr-Ca-Cu-O, Ba(Zn)-Fe-O, Mg-Fe-O, Mo-Si-O.

SOFTWARE ENGINEERING: Large-scale program design, Design of relational databases, Computer optimization of the technological flow.

PROGRAMMING: C++, Fortran, Java, Mathcad, ThermoCalc, Pandat, FACT, and Extend. **FOREIGN LANGUAGES:** *fluent*: English, Romanian, French, and Italian; *other*: Russian, Spanish.

AFFILIATIONS: Member of the American Physical Society, Materials Research Society, and American Nuclear Society.

WORK STATUS: Permanent resident of USA since 2000.

EDUCATION

Ph.D. (Physical Chemistry), March 1997, Thesis: “*Phase Diagram Calculation in Ceramic Oxide Systems*”, The Romanian Academy, Institute of Physical Chemistry, Bucharest, Romania. GPA: 4.00/4.00.

M.S. (Engineering Physics), June 1986, Thesis: “*The Electromagnetic Field Propagation in Nonlinear Media*”, University of Bucharest, Bucharest, Romania, GPA: 3.94/4.00.

WORK EXPERIENCE

10/1999-present **Technical Staff Member, Los Alamos National Laboratory, Materials Science and Technology Division:** Multi-scale modeling of physical and chemical properties of materials, phase diagram calculations, relational databases design, software engineering, and computer programming. PROJECTS (PI and Work Package Manager) *Advanced Fuel Cycle Initiative (AFCI)*: Models and simulations of phase stability, diffusion, and kinetics of chemical reactions in oxide, nitride and metallic nuclear fuels, *Enhanced Surveillance Campaign*: Modeling of Pu alloys phase stability and aging, *“Telluride” (ASCI, casting simulation software)*: Modeling of Materials Properties for Nuclear Fuels, *Mixed Oxides Fuels (MOX)*: Co-author of the Thermally Induced Gallium Removal (TIGR) process,

4/1997-10/1999 **Postdoctoral Research Associate, Los Alamos National Laboratory, Materials Science and Technology Division:** Modeling physical and chemical properties of nuclear materials, phase diagram calculations, relational databases design, computer programming, XRD, SEM, TEM. PROJECTS: Thermochemistry of MOX fuels, Thermal Induced Gallium Removal (TIGR) process, CO₂ sequestration.

10/1989-4/1997 **Research Scientist, Institute of Physical Chemistry**, Spl. Independentei. nr. 202, 77208, Bucharest, Romania: Studies on oxide materials, ceramics, superconductors, and phase equilibrium calculations.

9/1986-10/1989 **Head of the Physics Laboratory, ROFEP S. A.**, Urziceni, 8230, Romania: Computer optimization of technological flow, XRD, DTA, SEM, TEM, analysis and improvement of ferrite materials properties.

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Publications

Articles in Journals and Books (selection, in English)

- 1) M. Stan and P. Cristea, *Thermochemistry of Defects and Oxygen Diffusion in PuO_{2-x}*, submitted to J. Nucl. Mater., 2004.
- 2) P. Cristea and M. Stan, *Oxygen Diffusion in Nonstoichiometric Cerium Dioxide*, submitted to Phys. Rev. B, 2004.
- 3) P. Cristea and M. Stan, *Analytical Model of Defect Configurational Entropy of CeO(2-x) and PuO(2-x)*, submitted to J. Stat. Mech., 2004
- 4) M. Stan, Y. T. Zhu, H. Jiang, and D. P. Butt, *Kinetics of Oxygen Removal from Ceria*, J. Appl. Phys., **95** (2004) 3358-3361.
- 5) S. M. Valone, M. I. Baskes, M. Stan, T. E. Mitchell, A. C. Lawson, and K. E. Sickafus, *Simulations of Low Energy Cascades in fcc Pu Metal at 300 K and Constant Volume* J. Nucl. Mater., **324** (2004) 41-51.
- 6) M. Stan and B. J. Reardon, *A Bayesian Approach to Evaluating the Uncertainty of Thermodynamic Data and Phase Diagrams*, Calphad, **27** (2004) 319-323.
- 7) J. N. Mitchell, M. Stan, D. S. Schwartz, and C. J. Boehlert, *Phase Stability and Phase Transformations in Plutonium and Plutonium-Gallium Alloys*, Metall. Mater. Trans., **34A** (2004) 2267-2278.
- 8) M. I. Baskes, K. Muralidharan, M. Stan, S. M. Valone and F. J. Cherne, *Using the Modified Embedded-Atom Method to Calculate the Properties of Pu-Ga Alloys*, JOM, **55** (2003) 41-50.
- 9) M. I. Baskes and M. Stan, "An Atomistic Study of Solid/Liquid Interfaces and Phase Equilibrium in Binary Systems", Metal. Mater. Trans., **34A** (2003) 435-439.
- 10) M. I. Baskes, M. Stan, and K. Muralidharan, "Phase Stability of Pu and Pu-Ga Alloys from Atomistic Calculations", AIP Conf Proc, **673** (2003) 128-130.
- 11) M. Stan, T. J. Armstrong, D. P. Butt, T. C. Wallace, Sr., Y. Park, C. L. Haertling, T. Hartman, and R. J. Hanrahan Jr. "Stability of the Perovskite Compounds in the Ce-Ga-O and Pu-Ga-O Systems" J. Amer. Ceram. Soc., **85** (2002) 2811-2816.
- 12) D.G. Kolman, T.N. Taylor, Y.S. Park, M. Stan, D.P. Butt, C.J. Maggiore, J.R. Tesmer, and G.J. Havrilla, "Gallium Suboxide Attack of Stainless Steel and Nickel Alloys at 800°C to 1200°C", Oxid. Met., **55** (2001) 439-472.
- 13) D.G. Kolman, T.N. Taylor, Y.S. Park, M. Stan, D.P. Butt, C.J. Maggiore, J.R. Tesmer, and G.J. Havrilla "Gallium Suboxide Vapor Attack of Chromium, Cobalt, Molybdenum, Tungsten, and Their Alloys at 1200°C", Oxid. Met., **56** (2001) 347-374.
- 14) S. M. Valone, M. I. Baskes, M. Stan, and K. E. Sickafus, *Point-Defect Production and Migration in Pu Metal at Ambient Conditions*, Proceedings of the PRICM 4: Forth Pacific Rim International Conference on Advanced Materials And Processing, (2001) 2941-2943.
- 15) M. Stan, *Modeling the Thermodynamic Properties of Plutonium*, A. I. P. Conference Proceedings, **532** (2000) 390-391.
- 16) Y. T. Zhu, M. Stan, S. D. Cozone, and D. P. Butt, "Thermal Oxidation Kinetics of MoSi₂-Based Powders", J. Amer. Ceram. Soc., **82** (1999) 2785-2790.
- 17) M. Stan, "Phase Diagram Calculations in Materials Processing", in "Control and Optimization in Minerals, Metals and Materials Processing", Edited by the Canadian Institute of Mining, Metallurgy and Petroleum, Quebec, pp.161-169, 1999.
- 18) M. Stan, S.Mihaiu, D.Crisan, and M.Zaharescu, "Subsolidus Phase Equilibria in the Cu-Sb-O System", Eur.J.Solid State Inorg.Chem., **35** (1998) 243-254.

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- 19) M. Stan, A. Vasilescu, S. Moscu, and M. Zaharescu, "IR Structural Characterization of the Gels in the $\text{SiO}_2\text{-P}_2\text{O}_5$ System", Rev. Roum. Chim., **43** (1998) 425-432.
- 20) D. P. Butt, Y. Park, M. Stan, T. C. Wallace, Sr., R. H. Hanrahan, Jr., J. C. Huling, C. L. Haertling, D. G. Kolman, and C. A. James, "Thermal removal of Gallium from Weapons Plutonium Oxide", Proceedings of the Third Topical Meeting on DOE Spent Nuclear Fuel and Fissile Materials Management, September 8-11, 1998, Charleston, SC, Edited by the American Ceramic Society, Inc., pp. 556-557, 1998.
- 21) D. G. Kolman, C. A. James, D. P. Butt, Y. Park, and M. Stan, "Thermally-Induced Gallium Removal From Plutonium Dioxide For MOX Fuel Production", Proceedings of the Third Topical Meeting on DOE Spent Nuclear Fuel and Fissile Materials Management, September 8-11, 1998, Charleston, SC, Edited by the American Ceramic Society, Inc., pp. 558-559, 1998.
- 22) M. Stan, "On the Three-Factor Models and the Subregular Approximation in Phase Diagram Calculation", CALPHAD, **19** (1995) 169–178.
- 23) M. Stan, "Organizing a Relational System of Databases for Phase Diagram Calculation in Ceramic Oxide Systems", Proceedings of the Fourth EuroCeramics, "Basic Science", vol.2, p. 469-477, Edited by Gruppo Editoriale Faenza Editrice S. p. A., 1995.
- 24) A. Vasilescu, M. Stan, D. Crisan and R. Marchidan, "Sol-gel Materials in the $\text{TiO}_2 - \text{CdO}$ System" in "Zilele Academice Timisene", Ed. a IV-a, vol.1, pp.291-294, Ed. Mirton, Timisoara, 1995.
- 25) A. Vasilescu, M. Stan, R. Marchidan, and R. Popescu, "Sol - Gel Materials in the $\text{TiO}_2 - \text{Sb}_2\text{O}_3$ System", Proceedings of the 8th CIMTEC - World Ceramics Congress and Forum on New Materials, Florence, Italy, Edited by: P. Vicenzini, Faenza, 1995.
- 26) Teoreanu, V. Fruth, M. Zaharescu, G. Tanase, R. Popescu, M. Stan, and G. Aldica, "The Influence of Dopants on the Formation Mechanism of the Superconducting Phases in the Bi-Sr-Ca-Cu-O System", Proceedings of the Third EuroCeramics, vol.2, pp 659, Ed. P. Duran, 1993.
- 27) M. Zaharescu, M. Raileanu, S. Mihaiu, M. Stan, and L. Constantinescu, "Polysilicon Anions Polymerization Degree Determination", Rev. Chim., vol. **42** (1991) 406-410.

Scientific Reports

- 1) M. Stan, "The Thermodynamics and Kinetics of Truchas", Los Alamos National Laboratory Report, LA-UR-00-5749, 2000.
- 2) E. J. Luckwald and M. Stan, "Modeling the Excess Gibbs Free Energy of an Mg-Li Liquid Solution", Los Alamos National Laboratory Report, LA-UR-00-4709, 1999.
- 3) D. G. Kolman, Y. Park, M. Stan, R. J. Hanrahan Jr., and D. P. Butt, "An assessment of the Validity of Cerium Oxide as a Surrogate for Plutonium Oxide Gallium Removal Studies", Los Alamos National Laboratory Report, LA-UR-99-491, 1999.
- 4) D. P. Butt and M. Stan, "On the Maximum Acceptable Gallium Concentration in MOX Fuel: A Thought Exercise", Los Alamos National Laboratory Report, LA-UR-98-2854, 1998.
- 5) R. J. Hanrahan, S. L. Eaton, D. P. Butt, M. Stan, C. L. Haertling, and Y. Park, "Nuclear Fuels Technologies Fiscal Year 1998 Fuel Fabrication Development Gallium Sintering Summary Report", Los Alamos National Laboratory Report, LA-UR-98-4932, 1998.
- 6) K. M. Chidester, D. P. Butt, P. Chodak, S. F. DeMuth, S. L. Eaton, R. J. Hanrahan, G. J. Havrilla, C. L. Haertling, C. A. James, D. G. Kolman, A. D. Neuman, Y. Park, C. A. Smith, M. Stan, S. A. Talachy, J. G. Teague, H. R. Trellue, and C. J. Worley, "Nuclear Fuels Technologies Fiscal Year 1998 Research and Development Summary of Test Results", Los Alamos National Laboratory Report, LA-UR-98-5355, 1998.

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- 7) D. P. Butt, R. J. Hanrahan, Jr., Y. Park, and M. Stan, "Thermodynamics, Phase Relationships, and the Kinetics of Gallium Removal from Mixed Oxide Fuel Fabricated with Weapons Grade Plutonium", Los Alamos National Laboratory Report, LA-UR-97-4719, 1997.
- 8) D. P. Butt, R. J. Hanrahan, Jr., Y. Park, M. Stan, and T. C. Wallace, Sr., "Thermodynamics and Kinetics of Ga in MOX", Los Alamos National Laboratory Report, LA-UR-97-3853, 1997.
- 9) D. P. Butt, M. Stan, and D.G. Kolman, "Ga Issues in 3013 Containers", Los Alamos National Laboratory Report, LA-UR-97-2866, 1997.
- 10) M. Stan, "A Model for the Composition Modifications in the Cu-Sb-O System", Los Alamos National Laboratory Report, LA-UR-97-2020, 1997.
- 11) H. R. Trellue, T. Baros, H.T. Blair, J. J. Buksa, D. P. Butt, K. Chidester, S. F. DeMuth, S. L. Eaton, G. L. Havrilla, R. J. Hanrahan, Jr., C. A. James, D. G. Kolman, R. E. Mason, Y. Park, M. Stan, J. H. Steele, Jr., S. S. Vos, T. C. Wallace, Sr., C. G. Worley, "Nuclear Fuels Technologies Fiscal Year 1997 Research and Development Test Results", Los Alamos National Laboratory Report, LA-UR-97-4423, 1997.

Conference Presentations

- 1) M. Stan, *Models And Simulation of High Temperature Properties and Phenomena*, Gordon Research Conference on High Temperature Materials, Processes and Diagnostics, Waterville, ME, Aug. 1- 6, 2004.
- 2) M. Stan, S. Swaminarayan, and K. Lam, *Chemical Reaction Models in Truchas*, TRUCHAS Workshop, Los Alamos, NM, June 21-24, 2004.
- 3) B. Reardon and M. Stan, *Model Validation Methods for Phase Diagram Determination*, SAMO-Sensitivity Analysis and Model Output Conference, Santa Fe, NM, March 8-11, 2004.
- 4) M. Stan, P. Cristea, and T. C. Wallace, Sr., *Phase Stability, Diffusion, and Heat Transfer in Actinide Based Ceramics and Surrogate Materials*, MMSNF2 Workshop, New Orleans, LA, Nov. 20-21, 2003.
- 5) M. Stan, M. I. Baskes, and K. Muralidharan, *Phase Stability in the Pu-Ga System From First Principles and Molecular Dynamics Calculations*, 2003 MRS Fall Meeting, Boston, MA, Dec.1-5, 2003.
- 6) L. Popa-Simil, M. Hollander, D.R. Janecky, and M. Stan, *Dynamics of The Gas Production During He Ion Beam Bombardment of PTFE*, IBA-2003 Conference, Albuquerque, NM, July 1-4, 2003.
- 7) M. Stan, *Phase Stability and Phase Diagrams in the Pu-Ga System*, U.S. – Russian Plutonium Science Workshop, June 11, 2003, Los Alamos, NM, USA.
- 8) M. Stan, M. I. Baskes, S. P. Chen, and K. Muralidharan, *Phase Stability of Pu-Ga Alloys from First Principles and Molecular Dynamics Calculations*, XXXII CALPHAD Conference, La Malbay, Canada, May 25-30, 2003.
- 9) K. Muralidharan, M. I. Baskes, M. Stan, and S. G. Srinivasan, *Atomistic Modeling of the Phase Stability in the Pu-Ga System*, The 132nd TMS Annual Meeting & Exhibition, March 2-6, 2003, San Diego, CA, USA.
- 10) J. N. Mitchell, M. Stan, D. S. Schwartz, C. J. Boehlert, *Phase Transformations and Phase Stability in the Pu-Ga System*, The 132nd TMS Annual Meeting & Exhibition, March 2-6, 2003, San Diego, CA, USA.
- 11) Conference: 4th Pacific Rim International Conference on Advanced Materials and Processing (PRICM4); Honolulu, HI, Dec. 11-15, 2001.
- 12) S. M. Valone, M. I. Baskes, M. Stan, and K. E. Sickafus, "Radiation Damage in Pu Metals and Alloys", 23rd Aging, Compatibility, and Stockpile Stewardship Conference, Livermore, CA, November 14-16, 2000.

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- 13) J. C. Cooley, C. J. Boehlert, D. E. Dooley, J. N. Mitchell, M. Stan, and D. J. Thoma, "Phase Stability in Metastable Plutonium", 23rd Aging, Compatibility, and Stockpile Stewardship Conference, Livermore, CA, November 14-16, 2000.
- 14) M. Stan and B. Reardon, "A Bayesian Approach to Evaluating the Uncertainty of Thermodynamic Data and Phase Diagrams", CALPHAD XXX, York, UK, May 27 – June 1, 2001.
- 15) M. Stan, "The Perfect Thermodynamics of Imperfect Materials", CALPHAD XXX, York, UK, May 27 – June 1, 2001.
- 16) M. Stan, M. I. Baskes, S. M. Valone, and S. P. Chen , "Predicting Thermodynamic Properties of Materials", 2001 TMS Annual Meeting, New Orleans, LA, February 11-15, 2001.
- 17) M. I. Baskes, and M. Stan, "An Atomistic Study of Solid-Liquid Interfaces", 2001 TMS Annual Meeting, New Orleans, LA, February 11-15, 2001.
- 18) M. Stan, T. Armstrong, R. J. Hanrahan, Jr., D. P. Butt, T. C. Wallace, Sr., C. L. Haertling, and Y. Park
"Study of the Stability of a Perovskite Compound in the Pu(Ce)-Ga-O System", The 101 American Ceramic Society Conference, Indianapolis, IN, April 24-29, 1999.
- 19) M. Stan, "Phase Diagram Calculations in Materials Processing", The 38th Annual International Conference of Metallurgists, Quebec, Canada, August 22-26, 1999.
- 20) M. Stan , "Multi-Factor Models in Phase Diagram Calculations of Ceramic Oxide Systems", The 101 American Ceramic Society Conference, Indianapolis, IN, April 24-29, 1999.
- 21) M. Stan, D. P. Butt, and T. C. Wallace, Sr., "Phase Equilibrium Calculations in the Pu-Ga-O System", Third Pacific Rim International Conference on Advanced Materials and Processing, Honolulu, HI, July 12-16, 1998.
- 22) M. Stan and D. P. Butt, "Factorial Models In Phase Diagram Calculations of Ceramic Systems", The 50th Pacific Coast Regional and Basic Science Division Meeting of The American Ceramic Society, Irvine, CA, October 21-24, 1998.
- 23) D. P. Butt, Y. Park, M. Stan, T. C. Wallace, Sr., R. J. Hanrahan, Jr., J. C. Huling, C. L. Haertling, D. G. Kolman, and C. A. James, "Thermal Removal of Gallium from Weapons Grade Plutonium Oxide", American Nuclear Society Conference, Charleston, South Carolina, September 8-11, 1998.
- 24) M. Stan, T.C. Wallace, and D. P. Butt, "The Thermodynamics of Gallium Oxides in CeO_{2-x} and PuO_{2-x}", The 100 AcerS Conference, Cincinnati, OH, May 3-6, 1997.
- 25) M. Stan, "A Model for the Composition Modifications in the Cu-Sb-O System", 26th CALPHAD Conference, Palm Coast, FL, May 11-16, 1997.
- 26) M. Stan , "Organizing a Relational System of Databases for Phase Diagram Calculation in Ceramic Oxide Systems", The Fourth EuroCeramics Conference, Florence, Italy, June 29-July 4, 1995.
- 27) S. Moscu, and M. Stan , "IR Structural Characterization of the Sol-Gel Glasses in the SiO₂-P₂O₅ System", The National Conference of Physical Chemistry, Bucharest, Romania, September 21-23, 1994.
- 28) M. Stan, "On the Ternary Interaction Terms in Phase Diagram Calculation of Ceramic Oxide Systems", 8-th CIMTEC, Florence, Italy, 29 June-4 July, 1994.
- 29) A. Vasilescu, M. Stan, R. Marchidan, and R. Popescu, "Sol-Gel Materials in TiO₂-Sb₂O₃ System", 8-th CIMTEC, Florence, Italy, 29 June-4 July, 1994.
- 30) I.Toreanu, V.Fruth, M. Zaharescu, G. Tanase, M. Stan, and R. Popescu, "Some Preparation Aspects of Ceramic Materials with Superconducting Properties in the Bi-Sr-Ca-Cu-O System", Third EuroCeramics Conference, Madrid, Spain, September 12-17, 1993.

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- 31) I.Teoreanu, V.Fruth, M. Zaharescu, G. Tanase, M. Stan, and R. Popescu, "The Influence of Dopants on the Formation Mechanism of the Superconducting Phases in the Bi-Sr-Ca-Cu-O System", Third EuroCeramics Conference, Madrid, Spain, September 12-17, 1993.
- 32) M. Stan, "Subregular Models in Phase Diagram Calculations", The National Conference of Physical Chemistry, Bucharest, Romania, September 22-25, 1992.